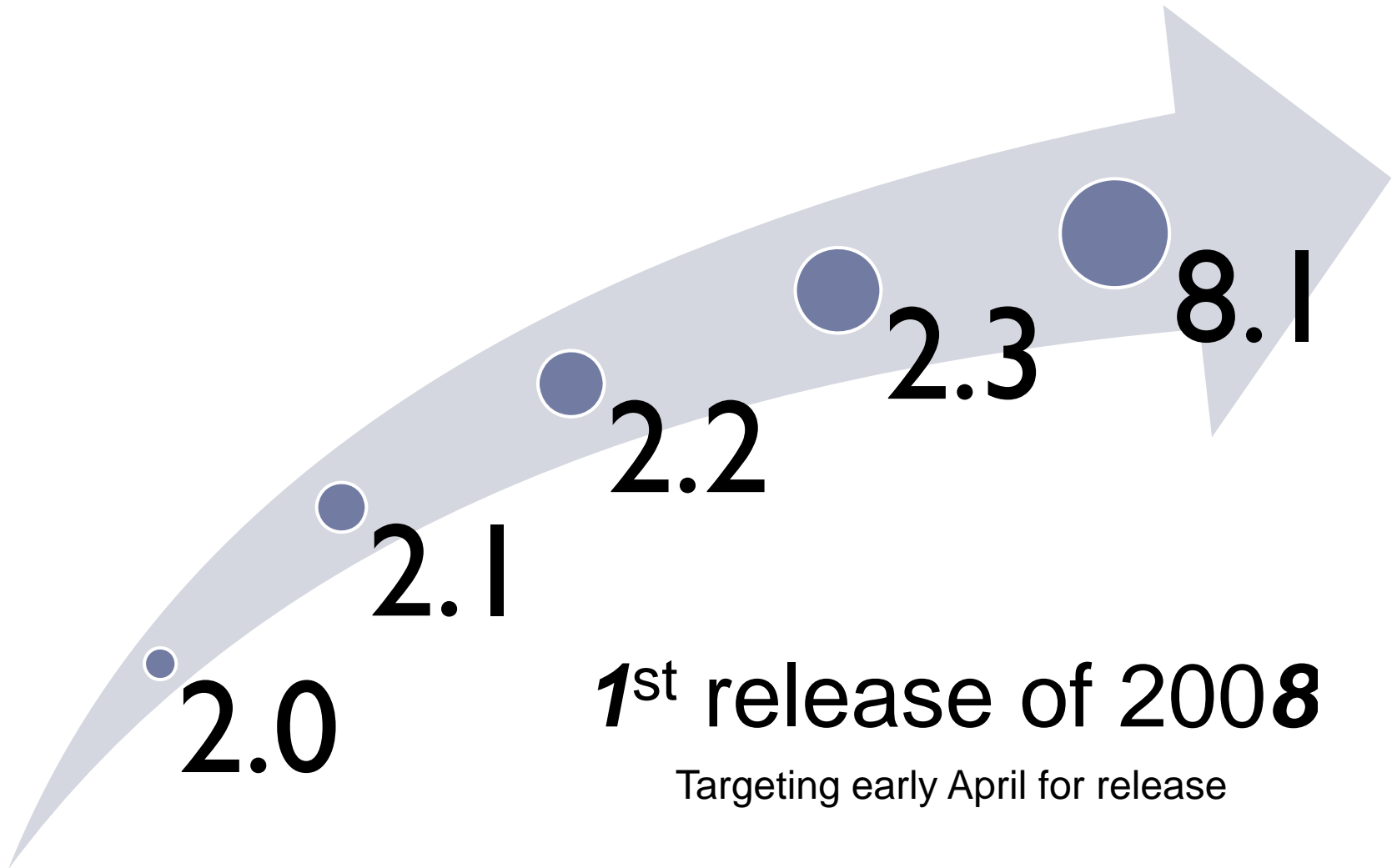


# What's New in LabKey CPAS 8.1

Josh Eckels and Peter Hussey

# Why 8.1?

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**1<sup>st</sup> release of 2008**

Targeting early April for release



LabKey software

## 8.1 New Features

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- ▶ **New assay types**
  - ▶ Elispot
  - ▶ Microarray
- ▶ **Javascript client API**
  - ▶ Build new user interfaces without writing Java code
  - ▶ Insert, update, and delete list data
  - ▶ Define custom reporting, charting
- ▶ **More flexible FTP server**
- ▶ **Many Flow Cytometry enhancements**
- ▶ **Many Study enhancements**



## 8.1 New Proteomics Features

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- ▶ Improved FASTA and Uni-Prot XML support
- ▶ Search for peptides
- ▶ MSI
  - ▶ Link MSI features and MS2 peptide identifications
  - ▶ Compare MSI runs
  - ▶ Search for MSI features
- ▶ Run groups for easily tagging and selecting runs
- ▶ Enhanced ProteinProphet comparison
- ▶ Label-free quantitation: Spectra Counting



# FASTA and Uni-Prot XML Improvements

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- ▶ Support for more FASTA files formats, including SGD
  - ▶ Extract more information, like gene names
  - ▶ Better organism identification
- ▶ Change the so-called “Best Name” to your choice of identifiers (IPI ,Swiss-Prot, etc)
- ▶ Choice of merging or replacing information when loading Uni-Prot XML files



Demo

# Label-Free Quantitation

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- ▶ Two approaches supported by CPAS 8.1
  - ▶ MS1/MS2 mapping
  - ▶ MS2 Spectrum counting
- ▶ Spectrum counting support
  - ▶ Visual display in CPAS
    - ▶ Example: Protein Prophet comparison
  - ▶ Datasets for consumption by scripts and tools
    - ▶ Example: Analysis via R Scripts
    - ▶ Example: Pivot tables in Excel



# Label-Free Quantitation in R

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- ▶ **Choose “Spectra Count” data set**
  - ▶ Desired level of grouping
    - ▶ peptide, protein, charge state
  - ▶ Filter as needed at peptide level
- ▶ **Customize Query for columns needed**
  - ▶ CPAS-calculated aggregates of measures
  - ▶ Custom annotation data
- ▶ **Example Data Set: PEPPeR from Broad**
  - ▶ Two mixes of 12 proteins, 25 runs each





# PEPPeR Example Data

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Name	Organism	Conc. In A	Conc. In B
Albumin	Cow	200	200
alpha-Casein S1	Cow	100	10
alpha-Casein S2	Cow	100	10
Aprotinin	Cow	100	5
beta-Galactosidase	E. Coli	1	10
beta-Lactoglobulin	Cow	50	1
Carbonic anhydrase	Cow	100	100
Fibrinogen beta chain	Cow	25	25
Myoglobin	Horse	100	100
Ovalbumin	Chicken	5	10
Plasminogen	Human	2.5	25
Ribonuclease	Cow	100	100
Transferrin	Human	10	5

- Loaded as custom protein list in CPAS
- Run groups defined for Alpha and Beta mix runs

# Label-Free Quantitation in R (con't.)

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- ▶ **R script integration in CPAS**
  - ▶ One data frame available as input to R
  - ▶ Multiple output formats (display and download)
  - ▶ Run interactively or as pipeline job
- ▶ **Tasks for spectral counting**
  - ▶ Break up single dataset into scoring inputs
  - ▶ Do scoring function, resulting in a data frame
    - ▶ Simple weighted totals
    - ▶ SASPECT example
    - ▶ Control over protein group reporting
  - ▶ Format one or more outputs
    - ▶ CPAS page, Excel download, R chart, etc.



# Label-free Quantitation in Excel

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- ▶ Start with peptide or protein grouping
- ▶ Export to Excel
- ▶ Invoke Pivot Table wizard
- ▶ Copy Pivot Table values to separate sheet
  - ▶ Do additional calculations , e.g. ratios
  - ▶ Do charts

